Iron-Based Superconductors As Odd Parity Superconductors

Jiangping Hu[1, 2]

[1]Beijing National Laboratory for Condensed Matter Physics,
Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China
[2]Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA

Parity is a fundamental quantum number to classify a state of matter. Materials rarely possess ground states with odd parity. We show that the superconducting state in iron-based superconductors is classified as an odd parity s-wave spin-singlet pairing state in a single trilayer FeAs/Se, the building block of the materials. In a low energy effective model constructed on the Fe square bipartite lattice, the superconducting order parameter in this state is a combination of a s-wave normal pairing between two sublattices and a s-wave η-pairing within the sublattices. Parity conservation was violated in proposed superconducting states in the past. The state has a fingerprint with a real space sign inversion between the top and bottom As/Se layers. The results demonstrate iron-based superconductors being a new quantum state of matter and suggest that the measurement of the odd parity can establish fundamental principles related to high temperature superconducting mechanism.

I. INTRODUCTION

Symmetry plays the central role in the search for beauty in physics. It controls the structure of matter and allows us to simplify a complicated problem. Gauge principle is a fundamental principle in physics. Models formulated in different gauge settings are equivalent. Symmetry and gauge principles together make the foundations of modern physics to solve complicated problems.

The recently discovered high temperature superconductors (high-T_c), iron-based superconductors[1–3], are layered materials with complicated electronic structures. The complexity causes a major difficulty in understanding pairing symmetry which arguably is the most important property and clue to determine pairing mechanism[4, 5].

In a strongly correlated electron system, major physics is determined locally in real space. Important properties, such as pairing symmetry in a superconducting state, are expected to be robust against small variation of Fermi surfaces in reciprocal space. Although superconducting mechanism related to high temperature superconductors (high T_c) is still unsettled, the robust d-wave pairing symmetry in cuprates[6] can be understood under this principle.

Is this principle still held for iron-based superconductors? Namely, do all iron-based superconductors possess one universal pairing state? Unlike cuprates, the answer to this question is highly controversial because different theoretical approaches have provided different answers and no universal state has been identified[5]. Nevertheless, as local electronic structures in all families of iron-based superconductors are almost identical and phase diagrams are smooth against doping[4, 5], it is hard to argue that the materials can approach many different superconducting ground states.

In conventional wisdom, there are several obvious requirements regarding electron pairing in superconducting states. First, pairing symmetry is known to be classified according to lattice symmetry. Second, in a uniform superconducting state, the total momentum for the Cooper pairs (modulo a reciprocal lattice vector) must be vanished. Finally, for a central symmetric lattice with a space inversion center, the parity of superconducting order parameters normally is even for a spin-singlet pairing and odd for a spin-triplet pairing[7]. These requirements are easily fulfilled in a system with a simple electronic structure, such as cuprates. However, for iron-based superconductors, they are highly non-trivial.

The unit cell in iron-based superconductors is intrinsically a 2-Fe unit cell while for simplicity, most theoretical models are effectively constructed based on an 1-Fe unit cell[8–13]. Obviously, these effective models have different lattice symmetry from the models defined on the original lattice. The difference may cause serious problems. For example, in the effective models, the pairings have been limited to two electrons with opposite momentum $(\vec{k}, -\vec{k})$, which we call it normal pairing in this paper, where $\vec{k}$ is momentum defined with respect to the 1-Fe unit cell in an iron square lattice. The momentum vector $Q = (\pi, \pi)$ is a reciprocal lattice vector in the original lattice with a 2-Fe unit cell. Thus, the pairings $(\vec{k}, -\vec{k}+Q)$, in principle, are also allowed according to the above second requirements. We will refer this pairing channel as an extended η-pairing[14, 15] and simply call it η-pairing in this paper. The possible existence of η-pairing was discussed in simplified models[16–18]. As order parameters are classified differently under different symmetry groups, we need to understand these orders under the original lattice symmetry. Otherwise, conseration laws could be violated.

In this paper, we show that the superconducting state in iron-based superconductors is a new state of matter which is classified as an odd parity s-wave spin-singlet pairing state in a single trilayer FeAs/Se, the building block of the materials. The superconducting states that were proposed in the past based on the effective d-orbital models of an iron square lattice are not parity eigenstates. Parity conservation was violated. We show that the su-

perconducting state which conserves parity includes both normal pairing between two sublattices of the iron square lattice and η-pairing within each sublattices. The states have a fingerprint with a real space sign inversion between the top and bottom As/Se layers. Our derivation is based on general symmetry and gauge requirements on the effective models for iron-based superconductors.

In the following, we first provide a complete symmetry analysis for pairing symmetries in iron-based superconductors. While the pairing symmetries can be classified according to D_{2d} point group at iron sites or C_{4v} point group at the center of an iron square, there are two types of pairing symmetries for a spin-singlet pairing state because of the intrinsic 2-Fe unit cell. They are distinguished from each other by opposite parity numbers. Second, we discuss the hidden symmetry properties of the effective models under the original lattice symmetry. We show that the effective hopping terms between two sublattices and within each sublattice have different symmetry characters. Third, we discuss a general gauge principle related to the definition of pairing symmetries and conclude that parity conservation was violated in the past. We provide the meanfield Hamiltonian in the new superconducting state and show that it can provide a unified description of all families of iron-based superconductors including both iron-pnictides[4] and iron-chalcognides[19–22]. Fourth, we discuss the smoking-gun experiments that can reveal the parity of the superconducting state. Finally, we discuss the fundamental impact on high T_c superconducting mechanism if it is confirmed.

Before we start the main content, we first make clear about a gauge setting for the effective models that were constructed based on all five iron d-orbitals[8–10]. In those effective models with an 1-Fe unit cell, a new gauge setting is taken[8–10], which effectively changes the momentum $\vec{k}$ to $\vec{k}+Q$ for d_{xz} and d_{yz} orbitals. In the following, without further clarification, the momentum $\vec{k}$ used in the definition of our normal pairing $(\vec{k},-\vec{k})$ and η-pairing $(\vec{k},-\vec{k}+Q)$ is the same momentum used in those papers rather than the momentum in a natural gauge setting.

II. SYMMETRY OF A SINGLE FE-AS(SE) TRILAYER

Iron-based superconductors are layered materials. The essential electronic physics is controlled by a single trilayer Fe-As(Se) structure, the building block of the superconductors. Although the coupling along c-axis between the building blocks has many interesting effects, the superconducting mechanism and the fundamental properties of the superconducting states, such as pairing symmetries, are expected to be solely determined within the single building block. The observation of superconductivity in a single FeSe layer grown by MBE has further justified this two-dimensional nature[20–22]. Therefore, we first focus on the study of a single Fe-As(Se) trilayer structure.

We start our analysis by understanding the lattice symmetry. As shown in Fig. 1, the structure has an inversion center, the origin, located at the middle of each Fe-Fe link. The unit cell with the origin at the center is marked by the shadowed area, which includes two irons and two As/Se atoms. We denote T as the translation group with respect to the unit cell. The symmetry group, thus, is described by a non-symmorphic space group $G = P4/nmm$[23]. The quotient group G/T is specified by 16 symmetry operations that include a space inversion $\hat{I}$. It is easy to check that these operations can be specified equivalently as $C_{4v} \oplus \hat{I}C_{4v}$ or $D_{2d} \oplus \hat{I}D_{2d}$, where C_{4v} is the point group with respect to the point at the middle of an iron square and D_{2d} is the point group defined at an iron site. It is important to note that both C_{4v} and D_{2d} are not defined with respect to the inversion center. Therefore, some symmetry operations in C_{4v} or D_{2d} are non-symmorphic. For example, the $\hat{C}_4$ rotation operation in C_{4v} is equivalent to $(\hat{C}'_4, \hat{t}_2)$, which represents $\hat{C}'_4$, an rotation $\frac{\pi}{2}$ along z-axis at the inversion center, followed by a translation operation $\hat{t}_2$ that translates $(\frac{1}{2}, \frac{1}{2}, 0)$ in the coordinate of an iron square lattice, a half of unit lattice cell along X direction labeled in Fig.1.

In summary, the full symmetry group can be written as

$$G/T = Z_2 \otimes D_{2d} = Z_2 \otimes C_{4v} \tag{1}$$

where $Z_2 = (\hat{E}, \hat{I})$. The group is a direct product of two subgroups which are defined with respect to different operation centers. $\hat{I}$ commutates with all symmetry operations in D_{2d} or C_{4v} in a sense that operations are considered to be identical if they only differ by a lattice transition with respect to the 2-Fe unit cell.

III. PARITY AND PAIRING SYMMETRY CLASSIFICATION

The pairing symmetry of a translation invariant superconducting state is classified by the IRs of G/T. If we ignore spin-orbital coupling, the ground state is expected to be a parity eigenstate. Since spin-singlet pairing is overwhelmingly supported experimentally in iron-based superconductors[4, 5], we focus on spin-singlet pairing states.

Conventionally, for a spin-singlet pairing state, the parity is even. However, due to the unit cell doubling, the parity operation here essentially takes mapping between two sublattices, A and B, in the iron square lattice as shown in Fig.1. Therefore there is no parity constraint for the pairing within each sublattice governed by D_{2d}. Thus, for each irreducible representation of D_{2d}, there are two different pairing states with opposite parities. The IRs of G/T are direct product of the IRs of two subgroups.

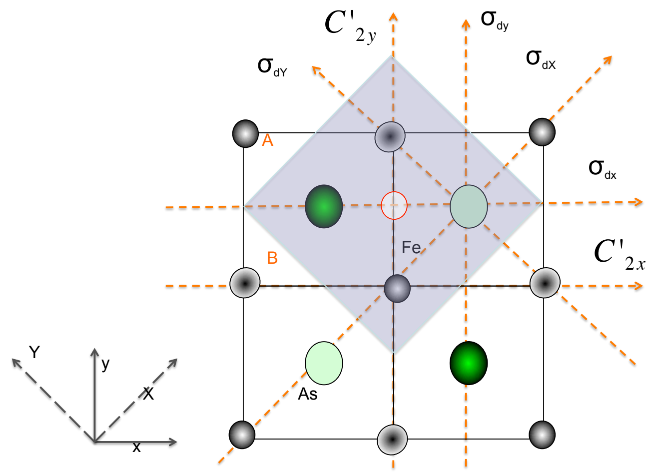

FIG. 1: Sketch of the lattice structure of a trilayer Fe-As(Se) unit. Notations used in the paper for axis directions, reflection symmetries and two sublattices are noted.

	E	$2S_4$	$C_2(z)$	$2C'_2$	$2\sigma_d$	Linear, rotations	Quadratic
A_1	1	1	1	1	1		x^2+y^2,z^2
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		x^2-y^2
B_2	1	-1	1	-1	1	z	xy
E	2	0	-2	0	0	(x,y) (R_x, R_y)	(xz,yz)

TABLE I: Character table for D_{2d} point group.

The character table of the D_{2d} group is shown in Table.I. There are five different IRs with four being one-dimensional, A and B, and one being two-dimensional, E. Let's consider the symmetry operation $\hat{S}_4^2$ in D_{2d}. It is easy to show that

$$\hat{I}\hat{S}_4^2 = (\hat{\sigma}_h, \hat{t}'_2), \tag{2}$$

where $\hat{\sigma}_h$ is the reflection along z-axis and $\hat{t}'_2$ is an in-plane translation by $(1,0,0)$, namely one iron-iron lattice distance. Eq.2 leads to an extremely important conclusion: The parity is determined by the eigenvalues of operation $(\hat{\sigma}_h, \hat{t}'_2)$. It is equal to or opposite to the eigenvalues for one-dimensional (A and B) or two-dimensional (E) IRs respectively because $\hat{S}_4^2 = 1$ for one-dimensional IRs and $\hat{S}_4^2 = -1$ for two-dimensional IRs. More specifically, this conclusion leads to that the pairing is translation invariant with respect to 1-Fe unit cell in the A or B state when the parity is even and in the E state when the parity is odd. The η-pairing takes place in the A or B state with odd parity and in the E state with even parity.

The above classification is independent of the number of orbitals and orbital characters as long as we have the gauge setting specified for d_{xz} and d_{yz} mentioned earlier.

It is also important to note that the classifications with respect to D_{2d} at iron sites or C_{4v} at the center of iron squares are equivalent in a sense that they can be mapped to each other. C_{4v} has the same number and type of IRs as D_{2d}. We notice the following important relation,

$$\hat{S}_4^3 = \hat{I}\hat{C}_4. \tag{3}$$

where $\hat{C}_4$ is the $\pi/2$ rotation operation in C_{4v}. For one-dimensional IRs in D_{2d}, the above equation reduces to $\hat{S}_4 = \hat{I}\hat{C}_4$. Therefore, for parity even pairing, namely normal pairing, there is no difference whether states are classified according to D_{2d} or C_{4v} since $\hat{S}_4 = \hat{C}_4$. Namely, a normal pairing state has the same IRs with respect to both C_{4v} and D_{2d}. For parity odd η-pairing, $\hat{S}_4 = -\hat{C}_4$, which implies that an s-wave state classified by A-IRs in D_{2d} must become an d-wave state classified by B-IRs in C_{4v}. For example, an η-pairing A_1 s-wave state classified in D_{2d} belongs to the B_2 d-wave in C_{4v}. Therefore, for an η-pairing parity odd state, the name of the state depends on how it is classified. For above example, one can either name the η-pairing state as B_{2u} d-wave or A_{1u} s-wave, depending on the classification point groups C_{4v} or D_{2d} respectively.

An odd parity superconducting state must have a sign change between the top and bottom As/Se layers. However, this information is hidden in an effective model with only d-orbitals constructed on an iron square lattice. From above symmetry analysis, we can track the parity information simply using $\hat{\sigma}_h$. Although $\hat{\sigma}_h$ is not a symmetry operation for a single Fe-As(Se) trilayer, the η-pairing state can be viewed as a state with *an internal negative iso-spin defined by* $\hat{\sigma}_h$. For any normal pairing, $\hat{\Delta}^n$ and η-pairing $\hat{\Delta}^\eta$ order parameters which belong to one-dimensional IRs of D_{2d}, we have

$$\hat{\sigma}_h \hat{\Delta}^n \hat{\sigma}_h = \hat{\Delta}^n \tag{4}$$

$$\hat{\sigma}_h \hat{\Delta}^\eta \hat{\sigma}_h = -\hat{\Delta}^\eta \tag{5}$$

We can extend above discussion for order parameters in a bulk material. There are two different lattice structures along c-axis in iron-based superconductors, 11-type (which includes 111($NaFeAs$) and 1111($LaOFeAs$) structures) and 122-type where the 11-type is translation invariant along c-axis while the 122-type is not.

For the 11-type, we can simply extend above analysis to the nearest-neighbour (NN) inter-layer pairing. For an even parity order parameters, we can have two possible terms: $(\vec{k}, -\vec{k})$ pairing which is proportional to $cos(k_z)$ and the η-pairing $(\vec{k}, -\vec{k}+Q)$ which is proportional to $isin(k_z)$. For an odd parity order parameters, the two possible terms become $(\vec{k}, -\vec{k})$ pairing which is proportional to $isin(k_z)$ and the η-pairing $(\vec{k}, -\vec{k}+Q)$ which is proportional to $cos(k_z)$. Both terms can be in a same irreducible representations of D_{2d}.

For the 122-type, the situation is rather different because the 122 structure has a symmorphic space group $I4/mmm$ with a point group D_{4h} centered in the middle of two NN Fe-As(Se) layers. The translation symmetry is specified by $(1,1,0)$, $(1,0,1)$, and $(0,1,1)$. The

space inversion and $\hat{\sigma}_h$ have identical characters in any one-dimensional IRs. A state with odd parity which belongs to one-dimensional IRs must have node lines on Fermi surfaces when $k_z = 0$. Therefore, we are only allowed to construct even parity states. For the intra-layer pairing, there are two different even parity order parameters: one is constructed by $(\vec{k}, -\vec{k})$ pairing and the other is constructed by $(\vec{k}, -\vec{k} + Q_3)$ pairing where $Q_3 = (\pi, \pi, \pi)$, namely the η-pairing. The difference between these two order parameters is that the latter breaks $(1, 0, 1)$ and $(0, 1, 1)$ translation symmetry. Now if we consider the NN inter-layer pairing, we can have two terms which are parity even and keep the translation symmetry: the normal pairing $(\vec{k}, -\vec{k})$ which is proportional to $cos(k_z)$ and $(\vec{k}, -\vec{k} + Q)$ pairing which is proportional to $isin(k_z)$. Here we refer $Q = (\pi, \pi, 0)$. For the $(\vec{k}, -\vec{k} + Q_3)$ η-pairing, there are also two terms in the NN inter-layer pairing: the η-pairing $(\vec{k}, -\vec{k} + Q_3)$ proportional to $cos(k_z)$ and $(\vec{k}, -\vec{k} + Q)$ pairing proportional to $cos(k_z)$. Therefore, if the inter-layer pairing is included, the superconducting state generally breaks translation symmetry of the iron-square lattice.

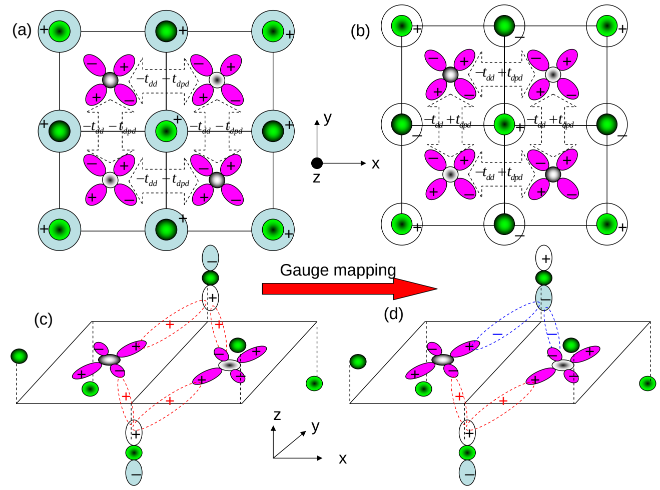

FIG. 2: (Color online) The nearest neighbor hopping parameters for intra-d_{xy}-orbital are shown in (a) and (b). t_{dd} is the amplitude of the direct hopping of d_{xy} orbital while t_{dpd} is the amplitude of the indirect hopping through p_z orbital of As/Se atom. The reason of sign change for t_{dpd} between (a) and (b) is that the p_z orbitals in top layer and bottom layer form occupied bonding states in (a) and empty anti-bonding states in (b). The difference is illustrated by filled and empty p_z orbitals in (a) and (b). (c) and (d) shows the local $p-d$ s-wave pairing pattern and the gauge transformation between them.

IV. EFFECTIVE HAMILTONIAN AND HIDDEN SYMMETRY

The above symmetry analysis is based on the original lattice symmetry. As we mentioned above, an effective model based on d-orbitals appears to have a different symmetry. In the past studies, we treated the model in 1-Fe unit cell with a D_{4h} point group at iron sites. The treatment, in general, violated the fundamental spirit of symmetry principle and might have resulted in fundamental errors. To pay a full respect to symmetry principle, we must understand the symmetry properties of the effective model under the original lattice symmetry.

We consider a general Hamiltonian in a single trilayer $Fe - As(Se)$ structure coordinated by Fe and As(Se) atoms,

$$\hat{H} = \hat{H}_{dd} + \hat{H}_{dp} + \hat{H}_{pp} + \hat{H}_I \tag{6}$$

where $\hat{H}_{dd}$, H_{dp} and $\hat{H}_{pp}$ describe the direct hopping between two d-orbitals, the $d-p$ hybridization between Fe and As(Se) and the direct hopping between two p-orbitals respectively. $\hat{H}_I$ describes any standard interactions. Here we do not need to specify the detailed parameters. This Hamiltonian has a full symmetry defined by the non-symmorphic space group.

An effective Hamiltonian is obtained by integrating out p-orbitals, which can be written as

$$\hat{H}_{eff} = \hat{H}_{dd,eff} + \hat{H}_{I,eff}. \tag{7}$$

The effective band structure can be written as $\hat{H}_{dd,eff} = \hat{H}_{dd} + \hat{H}_{dpd}$, where $\hat{H}_{dpd}$ is the effective hopping induced through d-p hybridization. $\hat{H}_{dd,eff}$ has been obtained by many groups[8–10, 24, 25]. The major effective hopping terms in $\hat{H}_{dpd}$ can be divided into two parts $\hat{H}_{dpd,NN}$, which describes NN hopping and $\hat{H}_{dpd,NNN}$, which describes NNN hoppings in the iron square lattice. If one carefully checks the effective hopping parameters for t_{2g} orbitals in $\hat{H}_{dpd,NN}$, one finds that they have opposite sign to what we normally expect in a natural gauge setting as shown in fig.2(a,b), where d_{xy} orbital is illustrated as an example. We see that the hopping parameter t_{dd} must be negative. However the effective hopping parameter, t_{dpd}, is positive and even larger than $|t_{dd}|$ in [8–10, 24, 25]. In a tetragonal lattice, t_{dpd} can only be generated through $d_{xy} - p_z$ hybridization. A positive value of t_{dpd} suggests that virtual hopping which generates t_{dpd} must go through an unoccupied p_z state. As shown in fig.2(a,b), a d_{xy} equally couples to p_z orbitals of top and bottom As atoms. A high energy p_z state must be an anti-bonding p_z state between NN As atoms. This analysis is held for all t_{2g} orbitals which play the dominating role in low energy physics. It is also easy to check that the effective NNN hoppings between t_{2g} orbitals are dominated through an occupied p states, which is primarily a bonding state of p -orbitals. Therefore, the NN effective hoppings are generated through $d-p_a$ hybridization, where p_a represents an anti-bonding p-orbital states and the NNN effective hoppings are generated through $d-p_b$ hybridization where p_b is the bonding p-state.

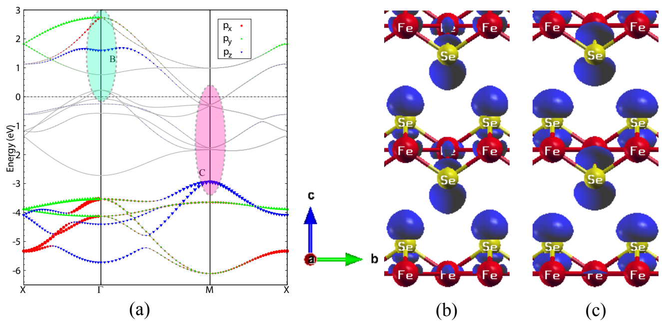

FIG. 3: (a) The calculated band structure of FeSe with the weight of p orbitals of Se. (b) The decomposed charge density of the band at Γ marked by letter B (anti-bonding states). (c)The decomposed charge density of the band at M marked by letter C (bonding states).

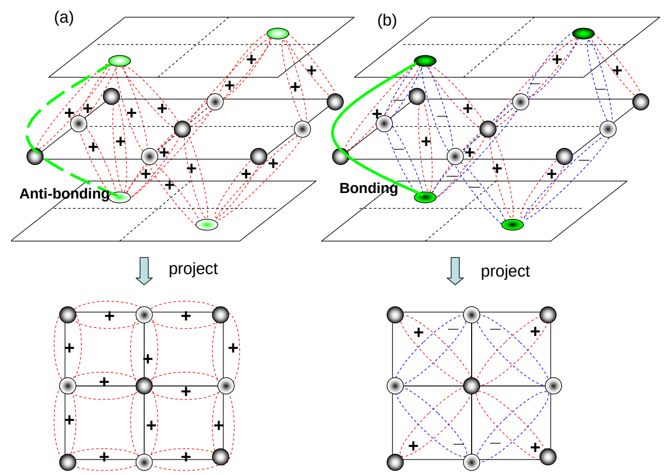

FIG. 4: (Color online) The NN and NNN $p-d$ local pairing patterns with odd parity are shown in (a) and (b) in the natural gauge. Note that p orbitals of As/Se in (a) form the anti-bonding states while that in (b) form the bonding states. We distinguish the two states with different filled green balls between (a) and (b). The $p-d$ pairings can be projected into effective $d-d$ pairings shown in the bottom row.

The above microscopic understanding is not surprising. In fact, it is known in LDA calculations[24, 26, 27] that p-orbitals in As/Se are not fully occupied and there are significant overlappings between p-orbitals on bottom and top As/Se layers. Moreover, since $\hat{H}_{dpd,NN}$ and $\hat{H}_{dpd,NNN}$ primarily affect hole pockets around Γ and electron pockets at M separately, we can check the distribution of anti-bonding p states and bonding p states in band structure to further confirm the analysis. In fig.3(a), we plot the band structure of FeSe and the distribution of p orbitals. The p_z orbitals of Se are mainly at +1.5 eV at Γ and -3 eV at M. By analyzing the bands at Γ and M as shown in Fig.3(b) and (c), we confirm that the p_z orbitals of Se at Γ and M belong to anti-bonding and bonding states separately.

Knowing the above hidden microscopic origins in a derivation of an effective Hamiltonian allows us to understand the symmetry characters of the effective Hamiltonian in the original lattice symmetry.

The $d-p_a$ hybridization is odd under $\hat{\sigma}_h$ while the $d-p_b$ hybridization is even under $\hat{\sigma}_h$. Thus, the NN hopping $\hat{H}_{dpd,NN}$ and NNN hopping $\hat{H}_{dpd,NNN}$ should be classified as odd and even under $\hat{\sigma}_h$ respectively. Namely,

$$\begin{aligned}\hat{\sigma}_h\hat{H}_{dpd,NN}\hat{\sigma}_h &= -\hat{H}_{dpd,NN} \\ \hat{\sigma}_h\hat{H}_{dpd,NNN}\hat{\sigma}_h &= \hat{H}_{dpd,NNN} \qquad (8)\end{aligned}$$

The above hidden symmetry property is against the main assumption taken in many weak coupling approaches, which assume that the essential physics is driven by the interplay between hole pockets at Γ and electron pockets at M [5]. As indicated in fig.3(a), the interplay between the hole and electron pockets must be minimal because of their distinct microscopic origins.

V. GAUGE PRINCIPLE AND PARITY CONSERVATION

The symmetry difference in eq.8 has fundamental impact on how to consider the parity of a superconducting state if superconducting pairing is driven by local d-p hybridization.

It has been shown that in a system where short range pairings in real space dominate, superconducting order parameters are momentum dependent and a gauge principle must be satisfied because the phases of superconducting order parameters can be exchanged with those of the local hopping parameters[16, 28] by gauge transformations. As an example, a d-wave superconducting state in cuprates can be mapped to a s-wave superconducting state by a gauge mapping which changes the hopping terms from s-type symmetry to d-type symmetry[29]. Therefore, only the combined symmetry of hopping terms and pairing orders associated to them is a gauge-independent symmetry character to classify superconducting states. Namely, the symmetry of a superconducting state is characterized by

$$Symmetry_{sc} = [\hat{H}_{hopping}][\hat{\Delta}] \qquad (9)$$

where $[\hat{A}]$ indicates the symmetry of $\hat{A}$. This gauge principle does not exist in a conventional BCS-type superconductor in which the information of pairing in real space is irrelevant.

Now we apply the gauge principle and let $\hat{\Delta}_{NN}$ and $\hat{\Delta}_{NNN}$ be superconducting order operators associated with $\hat{H}_{dpd,NN}$ and $\hat{H}_{dpd,NNN}$ respectively. In a superconducting state which belongs to a pure IR of the original lattice symmetry, we must have

$$[\hat{\Delta}_{NN}][\hat{H}_{dpd,NN}] = [\hat{\Delta}_{NNN}][\hat{H}_{dpd,NNN}] \qquad (10)$$

If we consider a superconducting state which conserves

parity, following eq.8, we have

$$[\hat{\Delta}_{NN}] = -[\hat{\Delta}_{NNN}] \tag{11}$$

under $\hat{\sigma}_h$. Therefore, based on the classification of pairing symmetries in Eq.5, a parity conserved superconducting state must be a combination of normal pairing and η-pairing. If $\hat{\Delta}_{NN}$ is a normal pairing, we immediately conclude that the state is parity odd and the superconducting order $< \hat{\Delta}_{NNN} >$ must be an η-pairing.

The above analysis can be easily illustrated in real space. As shown in fig.4, if superconducting pairing is driven by local d-p hybridization, the superconducting order is a pairing between d and p orbitals $\Delta_{dp} =< \hat{d}^{+}\hat{p}^{+} >$. A uniform $< \hat{d}^{+}\hat{p}_a^{+} >$ is parity odd. The NN pairing, $< \hat{\Delta}_{NN} >$ in the effective model, must originate from $< \hat{d}^{+}\hat{p}_a^{+} >$ and thus is also parity odd. The gauge principle can be understood as shown in fig.2(c,d). If we can take a new gauge for Fermion operators of p-orbitals, $\hat{p} \to -\hat{p}$, in one of the two As(Se) layers, the anti-bonding operator $\hat{p}_a$ maps to the bonding operator $\hat{p}_b$. This gauge mapping exactly transfers the parity between hopping terms and superconducting order parameters.

VI. MEANFIELD HAMILTONIAN FOR PARITY CONSERVED S-WAVE STATE

The above analysis can be generalized to all effective hoppings. The basic idea is to divide the iron square lattice into two sublattices. In an odd parity state, the pairing between two sublattices must be normal pairing while the pairing within sublattices must be η-pairing. In an even parity state, the pairing between two sublattices must be η-pairing while the pairing within sublattices must be normal pairing. This means that the pairing between two sublattices must be vanished in an even parity state.

In all of measured samples of iron-based superconductors, no universal node along $\Gamma - M$ and $\Gamma - X$ directions on all Fermi surfaces were observed[30–39]. These experimental facts place a constraint that the superconducting state must be in the A_1 IR of D_{2d}, namely, an s-wave viewed at iron sites. Then, the remaining question is about the parity of the state.

An even parity s-wave state, the normal pairing between two sublattices must be vanished. Therefore, the meanfield Hamiltonian for an even parity s-wave state is

$$H^e_{mf} = H_{dd,eff} + \sum_{\alpha,\beta,k} (\delta^e_{\alpha\beta,n} \hat{\Delta}_{\alpha\beta,n}(\vec{k}) + h.c.) \tag{12}$$

where $\hat{\Delta}_{\alpha\beta,n} = \hat{d}_{\alpha\uparrow}(\vec{k})\hat{d}_{\beta\downarrow}(-\vec{k}) - d_{\alpha\downarrow}(\vec{k})\hat{d}_{\beta\uparrow}(-\vec{k})$ and α, β label orbital. In general, the normal pairing order parameters must satisfy

$$\delta^e_{\alpha\beta,n}(\vec{k}) = \delta^e_{\alpha\beta,n}(\vec{k} + Q) \tag{13}$$

All superconducting states derived before from weak coupling approaches were considered as even parity[5, 8, 9, 40–43]. However, as a normal pairing between two sublattices is included, the parity is not conserved. In strong coupling models[44–47], the superconducting order was derived from NNN antiferromagnetic exchange coupling J_2, which is a normal pairing within sublattices, satisfies Eq.13. Therefore, if superconductivity is only originated from J_2, the proposed state is an even parity s-wave state, namely, the A_{1g} s-wave.

This state provides a good understanding of superconducting gaps in iron-based superconductors. However, it can not explain dual symmetry characters with both s-wave and d-wave type observed in the superconducting state, for example, the spin relaxation $\frac{1}{T_1 T}$ measured by nuclear magnetic resonance(NMR). A coherent peak around T_c is expected in a full gap s-wave state even if it is a $s^{\pm}$[5, 48]. Experimentally, in an extremely clean sample where the exponential temperature dependence was measured, no coherent peak was observed yet at T_c[49]. For iron-chalcogenides[19–22], this state is highly questionable because of the absence of sign change on Fermi surfaces so that it is hard to explain the possible sign change evidence from neutron scattering[50]. It is also worth mentioning that many weak coupling methods suggest that the superconducting state in iron-chalcogenides is a d-wave with normal pairing[18, 51, 52]. This state is not consistent with experimental results showing the absence of nodes on high symmetry lines[37–39] and the presence of strong ferromagnetic NN exchange coupling [53, 54]. Nevertheless, this d-wave state should be considered as an odd parity state in the original lattice symmetry because it only includes normal pairing between two sublattices.

A meanfield Hamiltonian to describe the odd parity s-wave state in 1-Fe unit cell (A_{1u} s-wave) can be generally written as

$$H^o_{mf} = H_{dd,eff} + \sum_{\alpha,\beta,k} (\delta^o_{\alpha\beta,n} \hat{\Delta}_{\alpha\beta,n}(\vec{k}) + \delta^o_{\alpha\beta,\eta} \hat{\Delta}_{\alpha\beta,\eta}(\vec{k}) + h.c.) \tag{14}$$

where $\hat{\Delta}_{\alpha\beta,\eta} = \hat{d}_{\alpha\uparrow}(\vec{k})\hat{d}_{\beta\downarrow}(-\vec{k}+Q) - \hat{d}_{\alpha\downarrow}(\vec{k})\hat{d}_{\beta\uparrow}(-\vec{k}+Q)$. In general, the normal and η pairing order parameters satisfy

$$\delta^o_{\alpha\beta,n}(\vec{k}) = -\delta^o_{\alpha\beta,n}(\vec{k} + Q) \tag{15}$$

$$\delta^o_{\alpha\beta,\eta}(\vec{k}) = \delta^o_{\alpha\beta,\eta}(\vec{k} + Q). \tag{16}$$

These equations capture the sign change of superconducting order parameters in momentum space. The sign change here is required by odd parity symmetry.

While detailed studies will be carried out in the future, the meanfield Hamiltonian captures superconducting gaps in both iron-pnictides and iron-chalcogenides. As the inter-orbital pairing can be ignored for s-wave pairing and the pairing is dominated by NN and NNN pairings, the important parameters are

$$\begin{aligned} \delta^o_{\alpha\alpha,n} &\propto cosk_x + cosk_y \\ \delta^o_{\alpha\alpha,\eta} &\propto cosk_x cosk_y. \end{aligned} \tag{17}$$

Thus, the superconducting gaps on hole pockets are mainly determined by $\delta^{o}_{\alpha\alpha,n}$ and those on electron pockets are mainly determined by $\delta^{o}_{\alpha\alpha,\eta}$.

In the odd parity s-wave state, there is no symmetry protected node. However, accidental nodes can easily take place. In fig.5, we plot numerical results for two cases. Parameters are specified in the caption of the figure. The superconducting gap in the first case is a full gap while it has gapless nodes on electron pockets in the second case. This may provide an explanation why gapless excitations were observed in some materials[5]. The detailed studies will be reported in future.

The odd parity s-wave state also explains the dual symmetry characters of both s-wave and d-wave type in iron-based superconductors. The η-pairing s-wave order in D_{2d} essentially is a d-wave type order according to C_{4v} as shown in Fig.4. For a d-wave pairing symmetry, the vanishing of the coherence factor is required by symmetry. Thus, current NMR results really support the odd parity state.

The Hamiltonian in Eq.14 can not be reduced to a translationaly invariant Hamiltonian in 1-Fe unit cell. The 2-Fe unit cell becomes intrinsic. Unique features related to 2-Fe unit cell should be observed and studied[55]. A detailed study will be carried out in future.

In summary, we provide the meanfield Hamiltonian for parity conserved superconducting states. Parity conservation was seriously violated in the past studies. Comparing odd and even parity s-wave states, we show that the odd parity s-wave state can naturally explain many intriguing properties of iron-based superconductors.

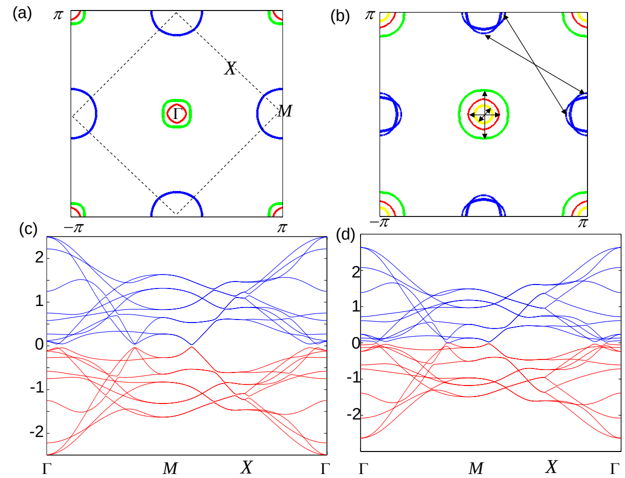

FIG. 5: (Color online) The Fermi surfaces of a five-orbital model in[25] are shown in (a) and (b). The forms of hopping terms and hopping parameters can be found in[25]. Here, we only add a chemical potentials to tune the fermi level. We set $\mu = 0.1$ and -0.04 in (a) and (b). The high-symmetry points are shown in (a) and the pairing channels connecting the points on the fermi surface are denoted by the black lines with arrows. The quasi-particle spectrum of the superconductive states for (a) and (b) are shown in (c) and (d). We can find the (c) is full gaped and (d) has nodes at the electron pockets. The superconductive order parameters are chosen: $\Delta^{N}_{11,x} = \Delta^{N}_{11,y} = 0.05$; $\Delta^{N}_{44} = 0.05$; $\Delta^{NN}_{11} = 0.05$; $\Delta^{NN}_{12} = 0.05$; $\Delta^{N}_{44} = -0.1$;

VII. SIGNATURE OF ODD PARITY SUPERCONDUCTING STATE

The fingerprint of the odd parity state is the negative iso-spin of $\hat{\sigma}_h$, which indicates the sign change of order parameters between top and bottom As(Se) layers. This property was first revealed in the recent constructed effective S_4 symmetry model based on the 2-Fe unit cell[16, 29, 56]. However, as the S_4 model is a simplified effective model based on two effective orbitals, the parity characters were not revealed.

The odd parity indicates that a superconducting single Fe-As(As) trilayer is a π-junction along c-axis, which can be measured in a single crystal material as shown in Fig.6: a uniform superconducting state is characterized by sign change between top and bottom surfaces along c-axis in 11-type structure while in the 122-type structure, the sign change only presents when the number of layers are odd.

VIII. DISCUSSION

In the history of condensed matter physics, a new quantum state of condensed matter is hardly obtained by solving a model. Here we use fundamental principles to show that an odd parity state can be naturally taken place in Iron-based superconductors and suggest smoking-gun experiments to detect or falsify it. With microscopic understanding proposed here, a detection of the odd parity state can have a tremendous impact on high T_c mechanism for iron-based superconductors and other high T_c superconductors.

In the past five years, many researches based on effective models suggest that pairing symmetries in iron-based superconductors are very fragile. Those studies essentially suggest that principles to understand the robustness of superconductivity and pairing symmetry are still missed in our standard approach. The results in this paper demonstrate that previous studies did not correctly take parity conservation and hidden symmetry in effective models into account and mishandled symmetry and gauge principles. In the past, the effective Hamiltonian was viewed in the symmetry group D_{4h} at iron sites rather than the original lattice symmetry G. We can see that if $\hat{\sigma}_h$ could be set to one, G is equivalent to D_{4h}. However, due to the anti-bonding p orbital states, the effective Hamiltonian does not represent correct symmetry of the original lattice in a natural gauge setting. It will be interesting to see how the missing pieces can be properly implemented in our standard methods.

Our results suggest that gauge principle needs to be properly implemented when we derive effective Hamiltonian to simplify a complex system. The correct physics can only be understood after the hidden gauge is revealed. For an order parameter which is momentum dependent, this gauge information is critical. The gauge principle becomes very important for us to search new physics in other complex electron systems.

The odd parity state also suggests the importance of correlated electron physics. It is believed that sign change superconducting order is inevitable in a superconducting state of strongly correlated electron systems because of the existence of strong repulsive interaction. This principle is violated in a parity even s-wave state. A measurement of the party odd s-wave state can provide a strong support of this principle.

The microscopic mechanism revealed here fundamentally differs from those proposed in weak coupling approaches which only emphasize Fermi surfaces. Fermi surfaces are only determined by energy dispersion. It provides no information about underlining microscopic processes which are local and bound with high energy physics. In correlated electron systems, these processes essentially determine many important properties. This is also the reason why iron-pnictides and iron-chalcogenides can be unified even if their Fermi surfaces are drastically different.

If the odd parity state is confirmed, the fundamental objects in superconducting states of high T_c materials must be the tightly binding Cooper pairs between d and p orbitals. In this view, the odd parity s-wave state closely resembles the d-wave state in a Cu-O plane of cuprates. We expect an identical mechanism to select sign changed superconducting orders in both materials. From Fig.4(b), one can see that the η-pairing part in the odd parity state can be viewed as two d-wave states formed in two sublattices, a direct analogy to the d-wave in cuprates.

This study opens a promising new direction for the research in iron-based superconductors and suggests that the physics in these materials is deeper and much more inspiring than what we realized before. It leaves many unanswered questions for us. A few questions are in order. First, what is relationship between magnetism and superconductivity? One can see that the collinear antiferromagnetic (C-AFM) state[57] observed in iron-pnictides has odd parity. This may partially answer why superconductivity and C-AFM order can coexist in the phase diagram. Second, what are other unique properties in an odd parity s-wave state? It is known that an odd parity p-wave state displays many unique properties. Third, what is the relationship between nematism and superconductivity? Nematism breaks rotational symmetry and was observed at high temperature[58]. Fourth, how robust is an odd parity state in response to impurity? Finally, this study points out that there are three possible scenarios related to parity in superconducting states, even, odd or broken. Experiments proposed here will finally nail down the truth. All the previous studies took even parity for granted without knowing that the parity was acturally broken in the proposed states. However, a parity breaking superconducting state is also an interesting state to explore.

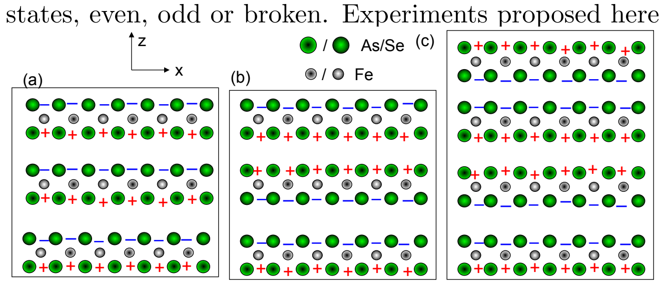

FIG. 6: Sketch of real space sign distribution along c-axis for an η-pairing state in (a) 11-type structure, (b) 122-type structure with odd number of layers and (c) 122-type structure with even number of layers.

In summary, using symmetry and gauge principles, we show that iron-based superconductors are unified into an odd parity s-wave superconducting state. We demonstrate that in an effective model based on d-orbitals, superconducting states studied in the past violate parity conservation. The existence of the odd parity state can have tremendous impact on high T_c superconducting mechanism.

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